Monte Carlo renormalization-group calculation for the $d = 3$ Ising model using a modified transformation

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We present a simple approach to high-accuracy calculations of critical properties for the three-dimensional Ising model, without prior knowledge of the critical temperature. The iterative method uses a modified block-spin transformation with a tunable parameter to improve convergence in the Monte Carlo renormalization group trajectory. We found experimentally that the iterative method enables the calculation of the critical temperature simultaneously with a critical exponent.

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I. INTRODUCTION

The Monte Carlo renormalization group (MCRG) method is a systematic procedure for computing critical properties of lattice spin models [1,2]. It is particularly flexible and can be applied to almost all lattice models, including percolation. MCRG is capable of excellent accuracy over a variety of models [3–12].

An important test case is the three-dimensional Ising model [13,14]. There are other methods that are capable of greater accuracy than MCRG for this model, but they are not as easily extended to treat more general models. The existence of these more specialized methods allows MCRG results to be tested against a true standard.

The three-dimensional Ising model is a particularly interesting test case. While the MCRG for the two-dimensional Ising model converges very rapidly, it has proved exceptionally difficult to achieve good results in three dimensions. A normal application of majority-rule RG transformation converges extremely slowly.

The key breakthrough was made by Blöte *et al.* [15] who used a three-parameter approximation to the fixed point, along with a modified majority rule for the RG transformation and showed dramatically improved convergence. Following this idea, we tuned the parameter involved in this modified rule more carefully and differently for different critical exponents [16].

All MCRG simulations start at a critical point (or, at least, at a good approximation of it), which is, unfortunately, not known for a general model nor for the three-dimensional Ising model. In this paper, we demonstrate a method for finding the critical coupling and a critical exponent simultaneously from a *single* simulation, without such a prior knowledge.

In the following section we recall the MCRG method. In Sec. III we review the tunable RG transformation. In Sec. IV we present our approach along with the results for the simultaneous calculations of the critical coupling and for y_{H1}. Finally, we present our conclusions and discuss future work.

II. MCRG COMPUTATIONS

The MCRG has often been reviewed [1,2,4,17], and here we only briefly outline the method. We consider the three-dimensional Ising model on a simple periodic cubic lattice, of size $N \times N \times N$. The Hamiltonian is given by

$$H = K \sum_{\langle j,k \rangle} \sigma_j \sigma_k, \tag{1}$$

where $\sigma_j = \pm 1$, and the sum is over all nearest-neighbor pairs. The dimensionless coupling constant K has been defined to include the inverse temperature $\beta = 1/k_B T$, so as to make the Boltzmann factor e^H.

The model was simulated using the Wolff algorithm [18] to generate a set of configurations characterizing the equilibrium distribution.

The renormalized configurations are obtained from these sets. For each configuration, the lattice is divided up into cubes, each containing eight sites, so that the scaling factor $b = 2$. A value of plus or minus 1 is assigned to each renormalized spin to represent the original spins in each cube in a way described below.

It is convenient to write the starting Hamiltonian (original simulated system) Eq. (1) in its most general form:

$$H^{(n)} = \sum_{\alpha} K_{\alpha}^{(n)} S_{\alpha}^{(n)}, \tag{2}$$

where the interactions S are combinations of the spins and the K's are the corresponding coupling constants. The sum is over

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all possible interactions that exist on a lattice of a given size. The subscript α denotes the type of interaction or coupling (nearest-neighbor, next-nearest-neighbor, four-spin, etc.). The superscript n is the number of applied renormalization steps. Since we have just described the first iteration of the renormalization transformation, $n = 1$. The nearest-neighbor coupling constant K defined earlier in Eq. (1), will also be denoted by $K_{nn}^{(0)}$. All other coupling constants at level $n = 0$ vanish.

To determine the critical exponents, we then need to calculate the matrix of derivatives of the couplings at level $n + 1$ with respect to the couplings at level n.

$$T_{\alpha,\beta}^{(n+1,n)} = \frac{\partial K_\alpha^{(n+1)}}{\partial K_\beta^{(n)}}. \tag{3}$$

This matrix of derivatives is then given by the solution of the equation

$$\frac{\partial \langle S_\gamma^{(n+1)} \rangle}{\partial K_\beta^{(n)}} = \sum_\alpha \frac{\partial \langle S_\gamma^{(n+1)} \rangle}{\partial K_\alpha^{(n+1)}} \frac{\partial K_\alpha^{(n+1)}}{\partial K_\beta^{(n)}}, \tag{4}$$

where

$$\frac{\partial \langle S_\gamma^{(n+1)} \rangle}{\partial K_\beta^{(n)}} = \langle S_\gamma^{(n+1)} S_\beta^{(n)} \rangle - \langle S_\gamma^{(n+1)} \rangle \langle S_\beta^{(n)} \rangle \tag{5}$$

and

$$\frac{\partial \langle S_\gamma^{(n+1)} \rangle}{\partial K_\alpha^{(n+1)}} = \langle S_\gamma^{(n+1)} S_\alpha^{(n+1)} \rangle - \langle S_\gamma^{(n+1)} \rangle \langle S_\alpha^{(n+1)} \rangle. \tag{6}$$

For our calculations we have included $N_o = 20$ odd interactions. We have followed [17], who calculated all 53 even and 46 odd interactions that fit in either a 3×3 square or a $2 \times 2 \times 2$ cube of spins, and used their first 20 odd interactions. The eigenvalues of the T matrix in Eq. (3) are found separately for the even and odd interactions. The largest odd eigenvalue exponent y_{H1} calculated below is then obtained from the largest eigenvalue of the odd T matrix by $y_{H1} = \ln\lambda/\ln 2$, as $b = 2$.

III. TUNABLE BLOCK-SPIN TRANSFORMATION

In [16], we showed that the usual majority rule, which performs well for the two-dimensional Ising model, converges very slowly for the three-dimensional Ising model.

So, instead of using the usual majority rule, the renormalized spin $\sigma'_\ell = \pm 1$, associated with ℓ, a $2 \times 2 \times 2$ cube of spins, was assigned a value according to the following probability [15]:

$$P(\sigma'_\ell) = \frac{\exp(w\sigma'_\ell \sum_{j\in\ell} \sigma_j)}{\exp(w \sum_{j\in\ell} \sigma_j) + \exp(-w \sum_{j\in\ell} \sigma_j)}. \tag{7}$$

For $w \to \infty$, this tends to the majority rule.

A special feature of this calculation is that the convergence of the RG transformation in Eq. (7) can be enhanced by optimizing the parameter w separately for each exponent. In [16], we determined the optimal value of w for the calculation of y_{T1} and y_{H1} much more carefully than in earlier work and showed its fast convergence compared with that of the majority rule. We found $w(y_{T1}) = 0.4314$ and $w(y_{H1}) = 0.555$. The determination of w for y_{T2} and y_{H2} turned out to need much more statistics. We observed that using the w obtained for y_{T1} (y_{H1}) also for the calculation of y_{T2} (y_{H2}), looked promising, but we believe that accuracy can still be enhanced.

The value of w was adjusted so that the sequence of calculated exponents would converge as fast as possible. That is, one may aim at vanishing differences $d_{n+1,n} = 0$,

$$d_{n+1,n} = \text{exponent}^{(n+1)} - \text{exponent}^{(n)} = 0, \tag{8}$$

where n denotes the number of RG iterations. Our final results showed little dependence of the exponent estimates on the number of RG iterations, and the very small fluctuations that remained did not appear to be systematic. We decided that an attempt to further reduce the errors was not promising.

It is important to note that there is nothing special in the form of Eq. (7) and thus it is possible to choose other parametrizations. An example is presented in the Appendix.

IV. TUNING THE BLOCK-SPIN TRANSFORMATION ALONG WITH THE INVERSE CRITICAL TEMPERATURE K_c

In [16], we used a known approximation to the critical inverse temperature $K_c = 0.221\,654\,4$ and showed that upon tuning the block-spin transformation parameter w, a faster convergence to the fixed point value of the critical exponent was achieved and hence better estimations for the critical exponent were obtained. Since for a general model the inverse temperature is usually unknown, we want to present a method in which both parameters, i.e., K_c and the optimal w, can be simultaneously calculated, thus enabling the fast extraction of the largest odd eigenvalue exponent y_{H1}. First, instead of using w [Eq. (7)], we use

$$u = \frac{1}{[1 + \exp(-4w)]}, \tag{9}$$

which behaves somewhat more linear than w as K_c is approached. We assume y_{H1} is a function of both K_c and u, i.e.,

$$y_{H1} = au + bu^2 + cK_c + duK_c + eu^2K_c + f. \tag{10}$$

We observed that while finding an optimal w, namely, a w for which $d_{n,n-1} = 0$ [see Eq. (8)], for the largest n we used, the value of $d_{n-1,n-2}$ at that w, was also very small. This was the case *only* when the known critical value of K_c was used. We experimentally show below that the two conditions $d_{n,n-1} = d_{n-1,n-2} = 0$ may jointly be used for determining K_c and u (and hence w), at least with very good accuracy. For large enough grids, more such conditions may be minimized by using least-square calculations as well as using a better approximation, such as

$$y_{H1} = au + bu^2 + cK_c + duK_c + eu^2K_c + f + gK_c^2. \tag{11}$$

We applied this approach to lattices 128^3 and 256^3. From six cases shown on the first six lines of Table I, we may calculate the six coefficients appearing in Eq. (10) separately for each $n = 2,\ 3,\ 4$, and 5. (The reliability of the six coefficients could, of course, be enhanced by least-square fitting to more than just six cases.) Then by demanding $d_{3,2} = d_{4,3} = d_{5,4} = 0$, a new pair of K_c and u (and hence w) is obtained by the Newton-Raphson method. See line 7 in Table I for lattice

TABLE I. The odd eigenvalue exponent y_{H1} calculated on lattice 128^3 by using the Wolff algorithm [18] with different values of K and u. n denotes the number of RG iterations.

	K	w	u	$n=5$	$n=4$	$n=3$	$n=2$
1	0.2216	0.5	0.8808	2.44676(12)	2.47269(7)	2.48294(3)	2.49179(2)
2	0.2216	0.6	0.9168	2.44690(14)	2.47009(6)	2.47648(3)	2.47887(2)
3	0.2216	0.7	0.9427	2.44725(14)	2.46895(6)	2.47335(3)	2.47158(2)
4	0.2217	0.5	0.8808	2.51531(13)	2.49572(6)	2.49065(2)	2.49430(2)
5	0.2217	0.6	0.9168	2.51190(15)	2.49178(5)	2.48378(2)	2.48133(1)
6	0.2217	0.7	0.9427	2.51031(14)	2.48999(5)	2.48041(2)	2.47397(2)
7	0.22165322	0.58819	0.9132	2.48122(10)	2.48181(4)	2.48096(2)	2.48131(1)
8	0.221654013	0.58674	0.912692	2.48167(10)	2.48199(4)	2.48110(2)	2.48147(1)
9	0.22165417	0.58628	0.912546				

size 128^3. Two additional iterations are shown in line 8 (9), where we used Eq. (11) for the first six lines together with line 7 (8, respectively). The resulting approximation for K_c is $K_c = 0.221\,654\,1(1)$ along with our estimation for $y_{H1} = 2.4819(1)$.

Table II shows similar results for lattice 256^3, where we also used $n = 6$ and the additional demand $d_{6,5} = 0$ and obtained $K_c = 0.221\,654\,7(1)$ and $y_{H1} = 2.4824(1)$.

Note that both tables show, as was demanded, smaller differences $d_{n,n-1}$, from one iteration to the other, for the relevant used values of n, supporting the stability and reliability of the calculation.

V. SUMMARY AND FUTURE WORK

The result of our computation for y_{H1} and a comparison with other works are shown in Table III. The agreement between the various methods is generally good, although some differences exist. Since we do not have estimates of the systematic errors in our results, we cannot really say what the source of the differences are. We presume that the difference between the current result for $y_{H1} = 2.4824(1)$ and our previous one $y_{H1} = 2.4829(2)$ [16], stems from the fact that different values for K_c were used in the two simulations. The most reliable of the estimates shown in Table III is that of Kos *et al.* [21], which uses the conformal bootstrap and the one calculated by Hasenbusch [19], which was a very careful Monte Carlo finite-size study that included many effects of corrections to scaling to provide limits on the systematic errors.

Our obtained estimate for $K_c = 0.221\,654\,7(1)$ is in agreement with $K_c = 0.221\,654\,4(3)$ [22], with $0.221\,654\,63(8)$ [19], and with $0.221\,654\,626(5)$ [23].

The main future work should of course be to extend the current method to fast calculation of critical properties of other models. As the Wolff algorithm is not general enough, we would like to develop an algorithm which would be based on the inverse RG simulations, which only involve simple Monte Carlo as presented in [10] and [11].

APPENDIX: OTHER PARAMETRIZATION

We present an example of a renormalization transformation which is not of the form of Eq. (7). For instance, one can parametrize $P(\sigma'_\ell)$ by

$$P(\sigma'_\ell = +1) = \begin{cases} 1 & \text{if } \sum_{j\in\ell}\sigma_j \geqslant 4 \\ w' & \text{if } \sum_{j\in\ell}\sigma_j = 2 \\ 0.5 & \text{if } \sum_{j\in\ell}\sigma_j = 0 \\ 1-w' & \text{if } \sum_{j\in\ell}\sigma_j = -2 \\ 0 & \text{if } \sum_{j\in\ell}\sigma_j \leqslant -4. \end{cases} \tag{A1}$$

Just to demonstrate this point, we did some tuning of the parameter w' for lattice size 128^3 at $K_c = 0.221\,654\,4$ [22]. We got for the odd eigenvalue exponent y_{H1} similar results to those obtained by using Eq. (7) as introduced in [16], e.g., the exponent we obtained for $N_o = 20$ after two renormalizations using $w' = 0.88$ was 2.4828(1), compared with 2.4829(2) there.

TABLE II. The odd eigenvalue exponent y_{H1} calculated on lattice 256^3 by using the Wolff algorithm [18] with different values of K and u. n denotes the number of RG iterations.

	K	w	u	$n=6$	$n=5$	$n=4$	$n=3$	$n=2$
1	0.2216	0.5	0.8808	2.37353(20)	2.44672(10)	2.47271(5)	2.48299(3)	2.4974(2)
2	0.2216	0.59	0.9137	2.37940(19)	2.44699(9)	2.47025(4)	2.47696(2)	2.7979(2)
3	0.2216	0.7	0.9427	2.38191(19)	2.44766(9)	2.46893(4)	2.47333(2)	2.47156(1)
4	0.2217	0.5	0.8808	2.57931(17)	2.51560(6)	2.49560(3)	2.49061(1)	2.49431(1)
5	0.2217	0.59	0.9137	2.57317(17)	2.51244(7)	2.49193(3)	2.48424(1)	2.48229(1)
6	0.2217	0.7	0.9427	2.56978(17)	2.51039(6)	2.49003(3)	2.48036(1)	2.47398(1)
7	0.221652674	0.58870	0.91331	2.47834(14)	2.48115(5)	2.48166(3)	2.48087(1)	2.48127(1)
8	0.221654712	0.58411	0.91185	2.48225(14)	2.48253(6)	2.48225(3)	2.48127(1)	2.48180(1)
9	0.221654781	0.58371	0.91172					

TABLE III. Estimates of the odd eigenvalue exponent y_{H1} from several sources. Values that are boldfaced are calculated to be consistent with the published exponents in the same source.

This work MCRG	Ref. [16] MCRG	Ref. [15] MCRG	Ref. [19] MC	Ref. [20] ϵ-expansion	Ref. [20] $d = 3$	Ref. [21] Conformal bootstrap
2.4824(1)	2.4829(2)	2.481(1)	**2.4819**(1)	**2.4820**(25)	**2.4833**(13)	**2.481851**(1)

[1] S.-K. Ma, Renormalization Group by Monte Carlo Methods, Phys. Rev. Lett. **37**, 461 (1976).

[2] R. H. Swendsen, Monte Carlo Renormalization Group, Phys. Rev. Lett. **42**, 859 (1979).

[3] R. H. Swendsen, Monte Carlo calculation of renormalized coupling parameters: I. $d = 2$ Ising model, Phys. Rev. B **30**, 3866 (1984).

[4] R. H. Swendsen, Monte Carlo calculation of renormalized coupling parameters: II. $d = 3$ Ising model, Phys. Rev. B **30**, 3875 (1984).

[5] R. Gupta, G. Guralnik, A. Patel, T. Warnock, and C. Zemach, Monte Carlo Renormalization Group for SU(3) Lattice Gauge Theory, Phys. Rev. Lett. **53**, 1721 (1984).

[6] R. Gupta, Monte carlo renormalization group: A review, in *Lattice Gauge Theory. NATO ASI Series*, edited by B. Bunk, K. Mütter, and K. Schilling (Springer, Boston, MA, 1986), Vol. 140, pp. 37–65.

[7] A. Brandt and D. Ron, Renormalization multigrid (RMG): Statistically optimal renormalization group flow and coarse-to-fine Monte Carlo acceleration, J. Stat. Phys. **103**, 231257 (2001).

[8] D. Ron and R. H. Swendsen, Calculation of effective Hamiltonians for renormalized or non-Hamiltonian systems, Phys. Rev. E **63**, 066128 (2001).

[9] D. Ron and R. H. Swendsen, The importance of multi-spin couplings in renormalized Hamiltonians, Phys. Rev. E **66**, 056106 (2002).

[10] D. Ron, R. H. Swendsen, and A. Brandt, Inverse Monte Carlo Renormalization Group Transformations for Critical Phenomena, Phys. Rev. Lett. **89**, 275701 (2002).

[11] D. Ron, R. H. Swendsen, and A. Brandt, Computer simulations at the fixed point using an inverse renormalization group transformation, Physica A **346**, 387 (2005).

[12] J.-H. Chung and Y.-J. Kao, Neural Monte Carlo Renormalization Group, Phys. Rev. Research **3**, 023230 (2021).

[13] H. W. J. Blöte and R. H. Swendsen, Critical behavior of the three-dimensional Ising model, Phys. Rev. B **20**, 2077 (1979).

[14] G. S. Pawley, R. H. Swendsen, D. J. Wallace, and K. G. Wilson, Monte Carlo renormalization-group calculations of critical behavior in the simple-cubic Ising model, Phys. Rev. B **29**, 4030 (1984).

[15] H. W. J. Blöte, J. R. Heringa, A. Hoogland, E. W. Meyer, and T. S. Smit, Monte Carlo Renormalization of the 3D Ising Model: Analyticity and Convergence, Phys. Rev. Lett. **76**, 2613 (1996).

[16] D. Ron, A. Brandt, and R. H. Swendsen, Surprising convergence of the Monte Carlo renormalization group for the $d = 3$ Ising model, Phys. Rev. E **95**, 053305 (2017).

[17] C. F. Baillie, R. Gupta, K. A. Hawick, and G. S. Pawley, Monte Carlo renormalization-group study of the three-dimensional Ising model, Phys. Rev. B **45**, 10438 (1992).

[18] U. Wolff, Collective Monte Carlo Updating for Spin Systems, Phys. Rev. Lett. **62**, 361 (1989).

[19] M. Hasenbusch, Finite size scaling study of lattice models in the three-dimensional Ising universality class, Phys. Rev. B **82**, 174433 (2010).

[20] R. Guida and J. Zinn-Justin, Critical exponents of the N-vector model., J. Phys. A: Math. Gen. **31**, 8103 (1998).

[21] F. Kos, D. Poland, D. Simmons-Duffin, and A. Vichi, Precision islands in the Ising and $O(N)$ models, J. High Energy Phys. 08 (2016) 036.

[22] A. L. Talapov and H. W. J. Blöte, The magnetization of the 3D Ising model, J. Phys. A: **29**, 5727 (1996).

[23] A. M. Ferrenberg, J. Xu, and D. P. Landau, Pushing the limits of Monte Carlo simulations for the three-dimensional Ising model, Phys. Rev. E **97**, 043301 (2018).